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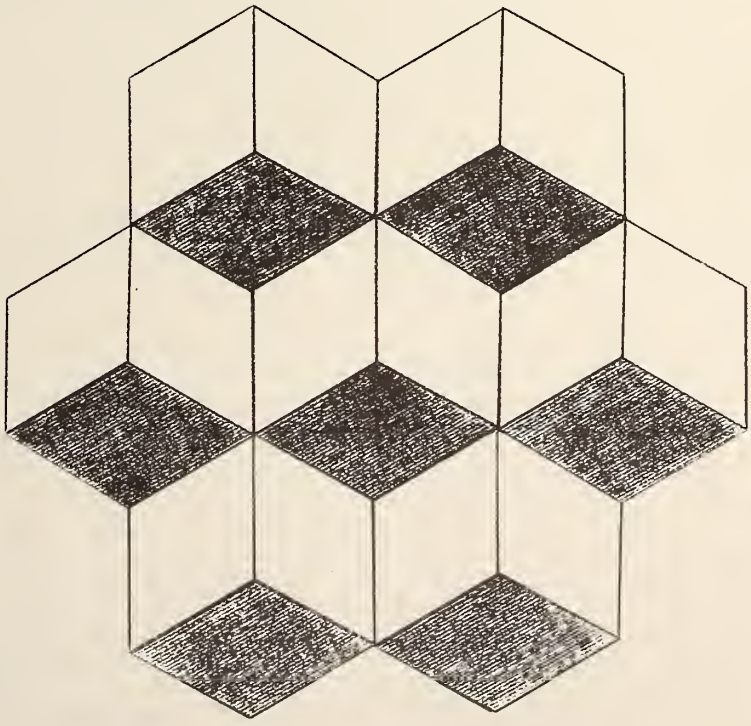
NIST ★ LATTICE
A Program to Analyze Lattice Relationships

Vicky Lynn Karen and Alan D. Mighell



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NIST ★ LATTICE
A Program to Analyze Lattice Relationships
Spring 1991 Version

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September 1991

*** Patent pending on certain algorithms used in this program. ***

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NIST*LATTICE
A Program to Analyze Lattice Relationships

I. Introduction

The NIST*LATTICE program is written in standard FORTRAN and is designed to be used in any analytical laboratory. The software is multifunctional and can be used to analyze various types of lattice relationships. The present version of the program performs several functions including : 1) the determination of symmetry, and the evaluation of experimental error, through Converse-Transformation analysis; 2) the generation of transformation matrices relating any two unit cells; 3) the calculation of the reduced cell of the lattice, and the calculation and reduction of specified derivative supercells and/or subcells; 4) unit cell transformations; and 5) matrix inversions. It is planned to incorporate additional features in forthcoming versions of this program.

II. RELATE TWO LATTICES via the Converse-Transform

A. General

This program function makes use of the Converse-Transformation operator, defined as

$$CT\,]_{h,t}\,(Y,Z) = \{\,(H,T)_{i,j}\,\}_{\substack{i=0,n \\ j=0,m}}$$

where h,t represent the domains of H,T, respectively, and Y,Z,H,T represent vector triples in R3 (Karen and Mighell, U.S. Patent Pending).

In this application of the CT operator, the REL program function allows the user to relate ANY two cells using the specified matrix elements, h, and input tolerances, t. Specifically, all transformation matrices, H, relating input CELL 2 to input CELL 1 are generated. The output tolerance matrix, associated with a matrix H, represents how closely the transformed CELL 2 agrees with CELL 1, and is of the form

tol a	tol b	tol c
tol alpha	tol beta	tol gamma

Thus, if CELL 2 is defined by A2, B2, C2, ALPHA2, BETA2, GAMMA2, then the transformation of CELL 2 by a matrix H will give a transformed cell having lattice parameters A1 + tol a, ... GAMMA1 + tol gamma.

B. Execution of program function

---

1) REL num probs

2)

I F M	range range num of elem	tol a	tol b	tol c	tol alpha	tol beta	tol gamma

3) a11 a12 a13 a21 a22 a23 a31 a32 a33
(M option only)

4)

(CELL 1)	A1	B1	C1	ALPHA1	BETA1	GAMMA1
(CELL 2)	A2	B2	C2	ALPHA2	BETA2	GAMMA2

(Lattice Group 1)

FORMATS

1)	PROGRAM Line	(A5,3X,I2)
2)	REL Line	(A1,2X,I2,5X,6F10.5)
3)	Possible matrix elements (format = MATRIX Line) (M-option only)	(9F8.2)
4)	CELL Line	(10X,6F10.5)

COMMENT

* Repeat (4) to equal number of problems.

* Relate cell with smaller volume to cell with larger volume; that is, set CELL 1 = large volume and CELL 2 = small volume (program calculates inverse matrix).

* Recommend routine use of I 8 or larger.

* CAUTION - Use F,M options with extreme caution. Start with small tolerances and restrict number of matrix elements input. If necessary, gradually increase with subsequent executions of the program.

III. Reduction and Derivative Lattice

A. General

The reduced cell is a unique, primitive cell that is based on the three shortest noncoplanar vectors of the lattice and satisfies a specified set of mathematical conditions. To be reduced, the cell must be in normal representation and both the main and the special conditions for reduction must be met.

Reduction is a mathematical procedure that leads to a unique cell, provided there is no experimental error in the unit cell parameters. Unfortunately, experimental error is always present for cells determined in the laboratory. Furthermore, it appears that the reported experimental error is too optimistic, even for unit cells refined by least-squares analysis using modern diffractometry. This is especially true when working with cells prior to the final cell, or for cases in which unit cell parameters were determined from irregularly shaped crystals having an absorption problem. Thus, it is essential that the symmetry and experimental error be evaluated through CT analysis BEFORE attempting to obtain a standard or conventional cell.

There are many reasons for calculating derivative cells of the lattice. For example, cells determined from single-crystal and powder data are sometimes derivative cells. In single-crystal work, a subcell in direct space may be determined if reciprocal lattice nodes are missed on a diffraction photograph or a diffractometer. When using powder methods, a supercell in direct space may be determined if one does not find the smallest cell consistent with a set of d-spacings. With NIST*LATTICE, supercells having volumes n (n = 2-9) times the volume of the reduced input cell and/or subcells having 1/n (n = 2-9) times the volume of the reduced input cell may be calculated.

B. Execution of program function

---

1) RSS num probs

2)

type	delta s	centering	A	B	C	ALPHA	BETA	GAMMA
					(cell)			

FORMATS

1) PROGRAM Line (A5,3X,I2)

2) RSS Line (I1,2X,2I1,3X,2A1,6F10.2)

COMMENTS

* Repeat (2) to equal number of problems.

* CAUTION - RSS alone should NOT be used to determine symmetry or to find a transformation matrix to a conventional cell.

IV. SYMMETRY DETERMINATION through Converse-Transformation Analysis

A. General

In sharp contrast to other methods which focus on the consequences of symmetry (such as dot products, d-spacings, etc.), this approach deals with symmetry in its most abstract form - represented as matrices. The basis of the SYM program function is to generate a group of matrices reflecting the holohedry of the lattice. This is accomplished through a specialized application of the Converse-Transformation operator, defined as

$$CT\,]_{h,t}\ (Y,Z) = \{\ (H,T)_{i,j}\ \}_{\substack{i=0,n \\ j=0,m}}$$

where h,t represent the domains of H,T, respectively, and Y,Z,H,T represent vector triples in R3 (Karen and Mighell, U.S. Patent Pending).

The SYM program function generates the matrices, H, that relate ANY primitive cell of the lattice to itself. In theory, it is the nature of the matrices themselves that defines the set to be analyzed (i.e., those defining a symmetry group). In practice, however, the usual result is that the tolerance matrices alone clearly define the groups and all that is required to determine metric lattice symmetry and pseudosymmetry is to count. The numbers of matrices for the seven lattice metric symmetries are: triclinic, 1; monoclinic, 2; orthorhombic, 4; rhombohedral, 6; tetragonal, 8; hexagonal, 12; and cubic, 24.

Generated with each symmetry matrix is a tolerance matrix of the form

tol a	tol b	tol c
tol alpha	tol beta	tol gamma

Simply by averaging the group of tolerance matrices, an error matrix is calculated that may be compared directly to the e.s.d.'s for the primitive cell. More importantly, this error matrix (= averaged tolerance matrix) may be used to calculate an idealized cell reflecting exact metric symmetry (i.e., idealized cell = A1 + avg.tol.a, ... GAMMA1 + avg.tol.gamma). By incorporating information from both sets of matrices, H and T, the idealized cell provides a unique means of evaluating experimental error based on ALL the symmetry operations of the lattice. This is crucial when determining standard or conventional cells.

When evaluating symmetry using CT analysis, the experimentalist need not rely solely on metric information. The group of H matrices may be viewed as sets of equivalent (h,k,l)'s represented in matrix form. Write the indices of a known reflection as a column matrix and premultiply by H to generate sets of reflections that should have equivalent intensities if the metric and crystal symmetry agree.

Once the symmetry and error have been evaluated, obtaining a transformation matrix to a standard or conventional cell may be accomplished either through analysis of the H matrices themselves, or by inputing the idealized cell reflecting exact metric symmetry into the RSS program function with subsequent Table look-up (*Note* This is possible ONLY after the symmetry and experimental error have been evaluated through CT analysis).

For additional details as well as discussions of other theoretical and practical applications in crystallography, see Acta Cryst. (1987). A43, 375-384.

Table 1a. Metric Classification

Reduced Form #	Matrix	
Monoclinic		
10, 14	$\begin{matrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{matrix}$	I
17	$\begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ -1 & -1 & -1 \end{matrix}$	I
20, 25	$\begin{matrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{matrix}$	I
27	$\begin{matrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{matrix}$	I
28	$\begin{matrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & 1 \end{matrix}$	I
29	$\begin{matrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{matrix}$	I
30	$\begin{matrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & -1 & 1 \end{matrix}$	I

Table 1a. Metric Classification - continued

Reduced Form #	Matrix	
Monoclinic		
33	-1 0 0 0 1 0 0 0 -1	I
34	-1 0 0 0 -1 0 0 0 1	I
35	1 0 0 0 -1 0 0 0 -1	I
37	1 0 0 0 -1 0 -1 0 -1	I
39	1 0 0 -1 -1 0 0 0 -1	I
41	-1 0 0 0 1 0 0 -1 -1	I
43	-1 0 0 0 -1 0 1 1 1	I

Table 1a. Metric Classification - continued

Reduced Form =	Matrix			
Orthorhombic				
8	-1 -1 -1	0 0 1	0 1 0	
	0 0 1	-1 -1 -1	1 0 0	I
	0 1 0	1 0 0	-1 -1 -1	
13	-1 0 0	0 -1 0	0 1 0	
	0 -1 0	-1 0 0	1 0 0	I
	0 0 1	0 0 -1	0 0 -1	
16	-1 0 0	0 -1 0	0 1 0	
	0 -1 0	-1 0 0	1 0 0	I
	1 1 1	0 0 -1	-1 -1 -1	
19	-1 0 0	-1 0 0	1 0 0	
	-1 0 1	0 0 -1	1 -1 0	I
	-1 1 0	0 -1 0	1 0 -1	
23	-1 0 0	-1 0 0	1 0 0	
	0 0 -1	0 0 1	0 -1 0	I
	0 -1 0	0 1 0	0 0 -1	
26	-1 0 0	-1 0 0	1 0 0	
	-1 1 0	0 -1 0	1 -1 0	I
	0 0 -1	-1 0 1	1 0 -1	
32	-1 0 0	-1 0 0	1 0 0	
	0 -1 0	0 1 0	0 -1 0	I
	0 0 1	0 0 -1	0 0 -1	

Table 1a. Metric Classification - continued

Reduced Form #	Matrix			
Orthorhombic				
36	-1 0 0	-1 0 0	1 0 0	
	0 -1 0	0 1 0	0 -1 0	I
	1 0 1	0 0 -1	-1 0 -1	
38	-1 0 0	-1 0 0	1 0 0	
	0 -1 0	1 1 0	-1 -1 0	I
	0 0 1	0 0 -1	0 0 -1	
40	-1 0 0	-1 0 0	1 0 0	
	0 -1 0	0 1 0	0 -1 0	I
	0 1 1	0 -1 -1	0 0 -1	
42	-1 0 0	-1 0 0	1 0 0	
	0 -1 0	0 1 0	0 -1 0	I
	1 1 1	0 -1 -1	-1 0 -1	

Table 1a. Metric Classification - continued

Reduced Form #	Matrix		
Rhombohedral			
2, 4	-1 0 0 0 0 -1 0 -1 0	0 -1 0 -1 0 0 0 0 -1	0 0 -1 0 -1 0 -1 0 0
	0 0 1 1 0 0 0 1 0	0 1 0 0 0 1 1 0 0	I
9	-1 1 0 -1 0 0 -1 0 1	-1 1 0 0 1 0 0 1 -1	0 -1 0 -1 0 0 0 0 -1
	0 -1 0 1 -1 0 0 -1 1	1 0 0 1 -1 0 1 0 -1	I
24	-1 0 0 0 -1 0 1 1 1	-1 0 0 0 0 -1 0 -1 0	-1 0 0 1 1 1 0 0 -1
	1 0 0 -1 -1 -1 0 1 0	1 0 0 0 0 1 -1 -1 -1	I

Table 1a. Metric Classification - continued

Reduced Form #	Matrix								
Tetragonal									
6	-1	-1	-1	-1	0	0	0	-1	0	0	0	-1
	0	0	1	0	-1	0	-1	0	0	1	1	1
	0	1	0	1	1	1	0	0	-1	0	-1	0
	0	0	1	0	1	0	1	1	1			
	-1	-1	-1	1	0	0	0	0	-1		I	
	1	0	0	-1	-1	-1	-1	0	0			
7	-1	-1	-1	-1	0	0	0	-1	0	0	0	-1
	0	0	1	0	0	-1	1	1	1	-1	0	0
	0	1	0	0	-1	0	-1	0	0	1	1	1
	0	0	1	0	1	0	1	1	1			
	-1	-1	-1	1	0	0	0	-1	0		I	
	1	0	0	-1	-1	-1	0	0	-1			
11	-1	0	0	-1	0	0	0	-1	0	0	-1	0
	0	-1	0	0	1	0	-1	0	0	1	0	0
	0	0	1	0	0	-1	0	0	-1	0	0	1
	0	1	0	0	1	0	1	0	0			
	-1	0	0	1	0	0	0	-1	0		I	
	0	0	1	0	0	-1	0	0	-1			
15	-1	0	0	-1	0	0	0	-1	0	0	-1	0
	0	-1	0	0	1	0	-1	0	0	1	0	0
	1	1	1	0	-1	-1	0	0	-1	0	1	1
	0	1	0	0	1	0	1	0	0			
	-1	0	0	1	0	0	0	-1	0		I	
	1	0	1	-1	-1	-1	-1	0	-1			

Table 1a. Metric Classification - continued

Reduced Form #	Matrix											
Tetragonal												
18	-1	0	0	-1	0	0	-1	0	0	-1	0	0
	-1	0	1	-1	1	0	0	-1	0	0	0	-1
	-1	1	0	0	0	-1	-1	0	1	0	-1	0
	1	0	0	1	0	0	1	0	0			
	0	0	1	1	-1	0	1	0	-1		I	
	1	-1	0	1	0	-1	0	1	0			
21	-1	0	0	-1	0	0	-1	0	0	-1	0	0
	0	-1	0	0	0	-1	0	0	1	0	1	0
	0	0	1	0	-1	0	0	1	0	0	0	-1
	1	0	0	1	0	0	1	0	0			
	0	-1	0	0	0	-1	0	0	1		I	
	0	0	-1	0	1	0	0	-1	0			

Table 1a. Metric Classification - continued

Reduced Form #	Matrix			
Hexagonal				
12	-1 -1 0 0 1 0 0 0 -1	-1 -1 0 1 0 0 0 0 1	-1 0 0 0 -1 0 0 0 1	-1 0 0 1 1 0 0 0 -1
	0 -1 0 -1 0 0 0 0 -1	0 -1 0 1 1 0 0 0 1	0 1 0 -1 -1 0 0 0 1	0 1 0 1 0 0 0 0 -1
	1 0 0 -1 -1 0 0 0 -1	1 1 0 -1 0 0 0 0 1	1 1 0 0 -1 0 0 0 -1	I
22	-1 0 0 0 -1 -1 0 0 1	-1 0 0 0 -1 0 0 1 1	-1 0 0 0 0 -1 0 -1 0	-1 0 0 0 0 1 0 1 0
	-1 0 0 0 1 0 0 -1 -1	-1 0 0 0 1 1 0 0 -1	1 0 0 0 -1 -1 0 1 0	1 0 0 0 -1 0 0 0 -1
	1 0 0 0 0 -1 0 1 1	1 0 0 0 0 1 0 -1 -1	1 0 0 0 1 1 0 -1 0	I

Table 1a. Metric Classification - continued

Reduced Form #	Matrix			
Cubic				
1	$\begin{matrix} -1 & 0 & 0 \\ -1 & 0 & 1 \\ -1 & 1 & 0 \end{matrix}$	$\begin{matrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{matrix}$	$\begin{matrix} -1 & 0 & 1 \\ -1 & 1 & 0 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} -1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & 0 & 1 \end{matrix}$
	$\begin{matrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ -1 & 0 & 1 \end{matrix}$	$\begin{matrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & -1 \end{matrix}$	$\begin{matrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{matrix}$	$\begin{matrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & -1 & 1 \end{matrix}$
	$\begin{matrix} 0 & -1 & 1 \\ 0 & -1 & 0 \\ 1 & -1 & 0 \end{matrix}$	$\begin{matrix} 0 & -1 & 1 \\ 0 & 0 & 1 \\ -1 & 0 & 1 \end{matrix}$	$\begin{matrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & -1 \\ 0 & 1 & -1 \\ 1 & 0 & -1 \end{matrix}$
	$\begin{matrix} 0 & 0 & 1 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & -1 \\ -1 & 1 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & -1 \\ 1 & 0 & -1 \\ 0 & 0 & -1 \end{matrix}$
	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{matrix}$	$\begin{matrix} 1 & -1 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 0 \end{matrix}$	$\begin{matrix} 1 & -1 & 0 \\ 1 & 0 & -1 \\ 1 & 0 & 0 \end{matrix}$
	$\begin{matrix} 1 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 1 & -1 \end{matrix}$	$\begin{matrix} 1 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & -1 & 0 \end{matrix}$	$\begin{matrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{matrix}$	I

Table 1a. Metric Classification - continued

Reduced Form #	Matrix			
Cubic				
3	$\begin{matrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{matrix}$	$\begin{matrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{matrix}$	$\begin{matrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{matrix}$
	$\begin{matrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{matrix}$	$\begin{matrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{matrix}$
	$\begin{matrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{matrix}$
	$\begin{matrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$
	$\begin{matrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{matrix}$
	$\begin{matrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{matrix}$	$\begin{matrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{matrix}$	I

Table 1a. Metric Classification - continued

Reduced Form #	Matrix			
Cubic				
5	$\begin{matrix}-1 & -1 & -1\\ 0 & 0 & 1\\ 0 & 1 & 0\end{matrix}$	$\begin{matrix}-1 & -1 & -1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{matrix}$	$\begin{matrix}-1 & -1 & -1\\ 1 & 0 & 0\\ 0 & 0 & 1\end{matrix}$	$\begin{matrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 1 & 1 & 1\end{matrix}$
	$\begin{matrix}-1 & 0 & 0\\ 0 & 0 & -1\\ 0 & -1 & 0\end{matrix}$	$\begin{matrix}-1 & 0 & 0\\ 1 & 1 & 1\\ 0 & 0 & -1\end{matrix}$	$\begin{matrix}0 & -1 & 0\\ -1 & 0 & 0\\ 0 & 0 & -1\end{matrix}$	$\begin{matrix}0 & -1 & 0\\ 0 & 0 & -1\\ 1 & 1 & 1\end{matrix}$
	$\begin{matrix}0 & -1 & 0\\ 1 & 1 & 1\\ -1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 0 & -1\\ -1 & 0 & 0\\ 1 & 1 & 1\end{matrix}$	$\begin{matrix}0 & 0 & -1\\ 0 & -1 & 0\\ -1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 0 & -1\\ 1 & 1 & 1\\ 0 & -1 & 0\end{matrix}$
	$\begin{matrix}0 & 0 & 1\\ -1 & -1 & -1\\ 1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 0 & 1\\ 0 & 1 & 0\\ -1 & -1 & -1\end{matrix}$	$\begin{matrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{matrix}$	$\begin{matrix}0 & 1 & 0\\ -1 & -1 & -1\\ 0 & 0 & 1\end{matrix}$
	$\begin{matrix}0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 1 & 0\\ 1 & 0 & 0\\ -1 & -1 & -1\end{matrix}$	$\begin{matrix}1 & 0 & 0\\ -1 & -1 & -1\\ 0 & 1 & 0\end{matrix}$	$\begin{matrix}1 & 0 & 0\\ 0 & 0 & 1\\ -1 & -1 & -1\end{matrix}$
	$\begin{matrix}1 & 1 & 1\\ -1 & 0 & 0\\ 0 & -1 & 0\end{matrix}$	$\begin{matrix}1 & 1 & 1\\ 0 & -1 & 0\\ 0 & 0 & -1\end{matrix}$	$\begin{matrix}1 & 1 & 1\\ 0 & 0 & -1\\ -1 & 0 & 0\end{matrix}$	I

Table 1b. Metric Classification

* CAUTION * The Reduced Form Matrix and Type must be calculated from the idealized cell reflecting exact metric symmetry.

Reduced Form No.	Reduced Form Matrix				Reduced Form Type	Bravais Lattice	Cell Transformation Reduced → Conventional
	First Row	Second Row					
	$a\cdot a\ b\cdot b\ c\cdot c$	$b\cdot c$	$a\cdot c$	$a\cdot b$			
a=b=c							
1	$a\cdot a\ a\cdot a\ a\cdot a$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Cubic F	$1\bar{1}1/11\bar{1}/\bar{1}11$
2	$a\cdot a\ a\cdot a\ a\cdot a$	$b\cdot c$	$b\cdot c$	$b\cdot c$	+	Rhombohedral hR	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
3	$a\cdot a\ a\cdot a\ a\cdot a$	0	0	0	-	Cubic P	100/010/001
4	$a\cdot a\ a\cdot a\ a\cdot a$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	-	Rhombohedral hR	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
5	$a\cdot a\ a\cdot a\ a\cdot a$	$-\frac{a\cdot a}{3}$	$-\frac{a\cdot a}{3}$	$-\frac{a\cdot a}{3}$	-	Cubic I	101/110/011
6	$a\cdot a\ a\cdot a\ a\cdot a$	$\frac{-a\cdot a+\lvert a\cdot b\rvert}{2}$	$\frac{-a\cdot a+\lvert a\cdot b\rvert}{2}$	$-\lvert a\cdot b\rvert$	-	Tetragonal I	011/101/110
7	$a\cdot a\ a\cdot a\ a\cdot a$	$-\lvert b\cdot c\rvert$	$\frac{-a\cdot a+\lvert b\cdot c\rvert}{2}$	$\frac{-a\cdot a+\lvert b\cdot c\rvert}{2}$	-	Tetragonal I	101/110/011
8	$a\cdot a\ a\cdot a\ a\cdot a$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot c\rvert$	$-(\lvert a\cdot c\rvert-\lvert b\cdot c\rvert-\lvert a\cdot c\rvert)$	-	Orthorhombic I	$\bar{1}\bar{1}0/\bar{1}0\bar{1}/0\bar{1}\bar{1}$
a=b							
9	$a\cdot a\ a\cdot a\ c\cdot c$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Rhombohedral hR	$100/\bar{1}10/\bar{1}\bar{1}3$
10	$a\cdot a\ a\cdot a\ c\cdot c$	$b\cdot c$	$b\cdot c$	$a\cdot b$	+	Monoclinic C**	$110/1\bar{1}0/00\bar{1}$
11	$a\cdot a\ a\cdot a\ c\cdot c$	0	0	0	-	Tetragonal P	100/010/001
12	$a\cdot a\ a\cdot a\ c\cdot c$	0	0	$-\frac{a\cdot a}{2}$	-	Hexagonal P	100/010/001
13	$a\cdot a\ a\cdot a\ c\cdot c$	0	0	$-\lvert e\cdot b\rvert$	-	Orthorhombic C	$110/\bar{1}10/001$
14	$a\cdot a\ a\cdot a\ c\cdot c$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot b\rvert$	-	Monoclinic C**	$110/\bar{1}10/001$
15	$a\cdot a\ a\cdot a\ c\cdot c$	$-\frac{a\cdot a}{2}$	$-\frac{a\cdot a}{2}$	0	-	Tetragonal I	100/010/112
16	$a\cdot a\ a\cdot a\ c\cdot c$	$-\lvert b\cdot c\rvert$	$-\lvert b\cdot c\rvert$	$-(a\cdot a-2\lvert b\cdot c\rvert)$	-	Orthorhombic F	$\bar{1}\bar{1}0/1\bar{1}0/112$
17	$a\cdot a\ a\cdot a\ c\cdot c$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot c\rvert$	$-(a\cdot a-\lvert b\cdot c\rvert-\lvert a\cdot c\rvert)$	-	Monoclinic I††	$\bar{1}0\bar{1}/\bar{1}\bar{1}0/011$
b=c							
18	$a\cdot a\ b\cdot b\ b\cdot b$	$\frac{a\cdot a}{4}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Tetragonal I	$0\bar{1}1/1\bar{1}\bar{1}/100$
19	$a\cdot a\ b\cdot b\ b\cdot b$	$b\cdot c$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Orthorhombic I	$\bar{1}00/0\bar{1}1/\bar{1}11$
20	$a\cdot a\ b\cdot b\ b\cdot b$	$b\cdot c$	$a\cdot c$	$a\cdot c$	+	Monoclinic C†	$011/01\bar{1}/\bar{1}00$
21	$a\cdot a\ b\cdot b\ b\cdot b$	0	0	0	-	Tetragonal P	010/001/100
22	$a\cdot a\ b\cdot b\ b\cdot b$	$-\frac{b\cdot b}{2}$	0	0	-	Hexagonal P	010/001/100
23	$a\cdot a\ b\cdot b\ b\cdot b$	$-\lvert b\cdot c\rvert$	0	0	-	Orthorhombic C	$011/0\bar{1}1/100$
24	$a\cdot a\ b\cdot b\ b\cdot b$	$-\frac{b\cdot b-\frac{a\cdot a}{3}}{2}$	$-\frac{a\cdot a}{3}$	$-\frac{a\cdot a}{3}$	-	Rhombohedral hR	$121/0\bar{1}1/100$
25	$a\cdot a\ b\cdot b\ b\cdot b$	$-\lvert b\cdot c\rvert$	$-\lvert a\cdot c\rvert$	$-\lvert a\cdot c\rvert$	-	Monoclinic C†	$011/0\bar{1}1/100$

Table 1b. Metric Classification (continued)

Reduced Form No.	Reduced Form Matrix				Reduced Form Type	Bravais Lattice	Cell Transformation Reduced → Conventional
	First Row†††	Second Row					
	a·a b·b c·c	b·c	a·c	a·b			
a≤b≤c 26	a·a b·b c·c	$\frac{a\cdot a}{4}$	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Orthorhombic F	100/$\bar{1}$20/$\bar{1}$02
27	a·a b·b c·c	b·c	$\frac{a\cdot a}{2}$	$\frac{a\cdot a}{2}$	+	Monoclinic I***	0$\bar{1}\bar{1}$/$\bar{1}$00/1$\bar{1}\bar{1}$
28	a·a b·b c·c	$\frac{a\cdot b}{2}$	$\frac{a\cdot a}{2}$	a·b	+	Monoclinic C	$\bar{1}$00/$\bar{1}$02/010
29	a·a b·b c·c	$\frac{a\cdot c}{2}$	a·c	$\frac{a\cdot a}{2}$	+	Monoclinic C	100/1$\bar{2}$0/00$\bar{1}$
30	a·a b·b c·c	$\frac{b\cdot b}{2}$	$\frac{a\cdot b}{2}$	a·b	+	Monoclinic C	010/01$\bar{2}$/$\bar{1}$00
31	a·a b·b c·c	b·c	a·c	a·b	+	Triclinic P	100/010/001
32	a·a b·b c·c	0	0	0	-	Orthorhombic P	100/010/001
33	a·a b·b c·c	0	-|a·c|	0	-	Monoclinic P	100/010/001
34	a·a b·b c·c	0	0	-|a·b|	-	Monoclinic P	$\bar{1}$00/00$\bar{1}$/0$\bar{1}$0
35	a·a b·b c·c	-|b·c|	0	0	-	Monoclinic P	0$\bar{1}$0/$\bar{1}$00/00$\bar{1}$
36	a·a b·b c·c	0	$-\frac{a\cdot a}{2}$	0	-	Orthorhombic C	100/$\bar{1}$0$\bar{2}$/010
37	a·a b·b c·c	-|b·c|	$-\frac{a\cdot a}{2}$	0	-	Monoclinic C*	102/100/010
38	a·a b·b c·c	0	0	$-\frac{a\cdot a}{2}$	-	Orthorhombic C	$\bar{1}$00/120/00$\bar{1}$
39	a·a b·b c·c	-|b·c|	0	$-\frac{a\cdot a}{2}$	-	Monoclinic C**	$\bar{1}\bar{2}$0/$\bar{1}$00/00$\bar{1}$
40	a·a b·b c·c	$-\frac{b\cdot b}{2}$	0	0	-	Orthorhombic C	0$\bar{1}$0/012/$\bar{1}$00
41	a·a b·b c·c	$-\frac{b\cdot b}{2}$	-|a·c|	0	-	Monoclinic C†	0$\bar{1}\bar{2}$/0$\bar{1}$0/$\bar{1}$00
42	a·a b·b c·c	$-\frac{b\cdot b}{2}$	$-\frac{a\cdot a}{2}$	0	-	Orthorhombic I	$\bar{1}$00/0$\bar{1}$0/112
43	a·a b·b c·c	$-\frac{b\cdot b-\lvert a\cdot b\rvert}{2}$	$-\frac{a\cdot a-\lvert a\cdot b\rvert}{2}$	-|a·b|	-	Monoclinic I	$\bar{1}$00/$\bar{1}\bar{1}\bar{2}$/0$\bar{1}$0
44	a·a b·b c·c	-|b·c|	-|a·c|	-|a·b|	-	Triclinic P	100/010/001

† If a·a < 4|a·c| } Premultiply Tabla Matrix by 00$\bar{1}$/010/101 (I centered)
* If b·b < 4|b·c| }
** If c·c < 4|b·c| }

†† If 3a·a < c·c + 2|a·c| } Premultiply Tabla Matrix by $\bar{1}$0$\bar{1}$/010/100 (C centered)
*** If 3b·b < c·c + 2|b·c| }

††† No required relationships between symmetrical scalars for reduced forms 26-44.

B. Execution of program function

---

1)	SYM	num probs					
2)	I R R1	range tol a	tol b	tol c	tol alpha	tol beta	tol gamma
3)	RSS Line information (only for R,R1 options)	A1	B1	C1	ALPHA1	BETA1	GAMMA1

FORMATS

1)	PROGRAM Line	(A5,3X,I2)
2)	SYM Line	(A1,I1.1X,I2,5X,6F10.5)
3)	CELL Line -- or -- RSS Line	(10X,6F10.5) (I1,2X,2I1,3X.2A1.6F10.2)

COMMENTS

* Repeat (3) to equal number of problems.

* Recommend routine use of large tolerances, typically 1.0 Angstroms and 4.0 degrees, in order to obtain a menu of all possible symmetries and pseudosymmetries.

* Recommend R option (large tolerances) for routine use, and I 24 option for skewed cells.

* For all executions except R or R1, a PRIMITIVE cell is assumed.

* For R, R1 matrix element codes, tolerances are applied to REDUCED cells

V. Cell Transformation

A. General

This program function enables the user to transform a unit cell by a specified three by three matrix. This transformation is defined by the equation :

(matrix) CELL A = CELL B ,

with a matrix of the form :

(a11 a12 a13)
(a21 a22 a23)
(a31 a32 a33)

B. Execution of program function

---

1) TRANS num probs

2) a11 a12 a13 a21 a22 a23 a31 a32 a33

3) A1 B1 C1 ALPHA1 BETA1 GAMMA1

FORMATS

1)	PROGRAM	Line	(A5,3X,I2)
2)	MATRIX	Line	(9F8.2)
3)	CELL	Line	(10X,6F10.5)

COMMENTS

* Repeat (2,3) to equal number of problems.

VI. Matrix Inversion

A. General

This program function enables the user to calculate the inverse of a three by three matrix of the form :

```
( a11  a12  a13 )
( a21  a22  a23 )
( a31  a32  a33 )
```

B. Execution of program function

---

1) INV num probs

2) a11 a12 a13 a21 a22 a23 a31 a32 a33

FORMATS

1)	PROGRAM	Line	(A5,3X,I2)
2)	MATRIX	Line	(9F8.2)

COMMENTS

* Repeat (2) to equal number of problems.

VII. Description of Input Lines

Each individual Section II through VI contains additional information concerning the theory and operations for each program function.

A. FORMATS

*	PROGRAM	Line	(A5,3X,I2)
*	CELL	Line	(10X,6F10.5)
*	MATRIX	Line	(9F8.2)
*	REL	Line	(A1,2X,I2,5X,6F10.5)
*	RSS	Line	(I1,2X,2I1,3X,2A1,6F10.2)
*	SYM	Line	(A1,I1,1X,I2,5X,6F10.5)

B. PROGRAM Line

The PROGRAM Line specifies the type of program function and the number of independent problems to be considered.

PROGRAM Line
Format(A5,3X,I2)

Column	Format	Item
1-5	A5	Type of program function 'REL ' = Relate Two Lattices 'RSS ' = Reduction and Derivative Supercell and Subcell 'SYM ' = Symmetry Determination 'TRANS' = Cell Transformation 'INV ' = Matrix Inversion
6-8	3X	Blank
9-10	I2	Number of problems

C. CELL Line

This input line is used to define a unit cell. All six unit cell parameters must always be specified regardless of the crystal symmetry.

CELL Line
Format(10X,6F10.5)

Column	Format	Item
1-10	10X	Blank
11-20	F10.5	a (Angstroms)
21-30	F10.5	b
31-40	F10.5	c
41-50	F10.5	alpha (degrees)
51-60	F10.5	beta
61-70	F10.5	gamma

D. MATRIX Line

The MATRIX Line defines the three by three matrix to be used when executing the TRANS or INV program functions.

MATRIX Line
Format(9F8.2)

Column	Format	Item
1-8	F8.2	Matrix element a11
9-16	F8.2	Matrix element a12
17-24	F8.2	Matrix element a13
25-32	F8.2	Matrix element a21
33-40	F8.2	Matrix element a22
41-48	F8.2	Matrix element a23
49-56	F8.2	Matrix element a31
57-64	F8.2	Matrix element a32
65-72	F8.2	Matrix element a33

E. REL Line

The REL Line defines the limits for the matrix elements and unit cell tolerances.

REL Line
Format(A1,2X,I2,5X.6F10.5)

Column	Format	Item
1	A1	I/F/M/ Matrix elements to be considered by the program I = Integers generated F = Integers generated plus fractions M = Manual input
2-3	2X	Blank
4-5	I2	1-40/1-10/2-99/ for I,F,M options I,F options = Range of integers generated M option = Number of matrix elements input
6-10	5X	Blank
11-20	F10.5	tol a
21-30	F10.5	tol b
31-40	F10.5	tol c
41-50	F10.5	tol alpha
51-60	F10.5	tol beta
61-70	F10.5	tol gamma

F. RSS Line

The RSS Line defines the input lattice and the derivative lattices to be calculated. The lattice is defined by specifying the cell centering and all six unit cell parameters.

RSS Line
Format(I1,2X,2I1,3X,2A1,6F10.2)

Column	Format	Item
1	I1	Blank/1/2/3/ Blank = Reduction 1 = Reduction + supercells 2 = Reduction + subcells 3 = Reduction + supercells, subcells
2-3	2X	Blank
4	I1	Blank/2/3/4/5/6/7/8/9/ Initial value (n1) to define the range of volumes for calculated derivative lattices.
5	I1	Blank/2/3/4/5/6/7/8/9/ Final value (n2) to define the range of volumes for calculated derivative lattices.
6-8	3X	Blank
9	A1	P/A/B/C/F/I/R/ Cell centering
10	A1	R/H/ Rhombohedral/Hexagonal/ metric axes. Used only for rhombohedral lattices.
11-20	F10.2	a (Angstroms)
21-30	F10.2	b
31-40	F10.2	c
41-50	F10.2	alpha (degrees)
51-60	F10.2	beta
61-70	F10.2	gamma

G. SYM Line

The SYM Line defines the limits for the matrix elements and unit cell tolerances, as well as the type of lattice transformations to be performed (i.e., the calculation and analysis of reduced and/or derivative lattices).

SYM Line
Format(A1,I1,1X,I2,5X,6F10.5)

Column	Format	Item
1	A1	I/R/ I = Integers generated R = RSS, then integers generated
2	I1	Blank/1/ Normal/abbreviated RSS output
3	1X	Blank
4-5	I2	1-40/ Range of integers generated
6-10	5X	Blank
11-20	F10.5	tol a
21-30	F10.5	tol b
31-40	F10.5	tol c
41-50	F10.5	tol alpha
51-60	F10.5	tol beta
61-70	F10.5	tol gamma

VIII. Program Execution: Example

A. Input flowstream

```
 1)  SYM      1
 2)  R         1.0       1.0       1.0       4.0       4.0       4.0
 3)  0  00   C 14.259    22.539    8.741     90.00     114.10    90.00
 4)  RSS      2
 5)  1  22   P 13.595    4.638     10.321    90.00     98.28     90.000
 6)  2  22   P 15.928    4.623     18.271    90.00     105.58    90.000
 7)  REL      1
 8)  F  10     0.2       0.2       0.2       1.0       1.0       1.0
 9)            6.003     6.007     23.389    97.04     92.61     110.16
10)            6.030     11.471    11.711    94.72     97.72     99.49
11)  TRANS    1
12)  -1.0    .00     .00     .50     .50     .00     -.5     -.5     -2.0
13)            6.030     11.471    11.711    94.72     97.72     99.49
14)  INV      2
15)  -1.0    .00     .00     .50     .50     .00     -.50    -.50    -2.0
16)  -1.0    .00     .00     1.0     2.0     .00     .00     -.50    -.50
```

Notes:

1 The 'SYM ' in columns 1-5 indicates that the SYM program function will be executed. The ' 1' in columns 9-10 specifies that one independent problem is to be considered.

2 The 'R ' in columns 1-2 instructs the program first to reduce the cell, with normal RSS output, and then to generate the symmetry matrices. The tolerances for the cell edges and angles are 1.0 Angstroms and 4.0 degrees, respectively.

3 This RSS Line instructs the program to calculate the reduced cell of a C-centered input cell. Regardless of the symmetry, all six unit cell parameters are specified in columns 11-70. Decimal numbers have been used for fractions of a degree.

4 The 'RSS ' in columns 1-5 indicates that the RSS program function will be executed; the ' 2' in columns 9-10 specifies that two RSS Lines will follow (two problems are to be considered).

5 The '1' in column 1 specifies that supercells will be calculated. The '22' in columns 4-5 are integers (n1 and n2) that define the range of volumes for derivative cells to be calculated. In this case, the supercells will have volumes ranging from (n1)V to (n2)V. All six unit cell parametes are given given in columns 11-70.

6 The '2' in column 1 specifies that subcells will be calculated. The '22' in columns 4-5 are integers (n1 and n2) that are used to define the range of volumes for the derivative cells to be calculated. The subcells will have volumes ranging from (1/n1)V to (1/n2)V.

7 The 'REL ' in columns 1-5 indicates that the REL program function will be executed. The ' 1' in columns 9-10 specifies one problem.

8 The 'F' in column 1 and the '10' in columns 4-5 specify that only integers in the range -10 to +10 plus simple rational numbers will be considered as possible matrix elements. The tolerances for the cell edges and angles are 1.0 Angstroms and 4.0 degrees. respectively.

9-10 The program will calculate the H matrices relating the two cells.

11 The 'TRANS' in columns 1-5 indicates that the TRANS program function will be executed. The ' 1' in columns 9-10 specifies that one independent problem will be considered.

12 This input line defines the matrix to be used to transform the input cell. Each matrix element has been specified by a decimal number.

13 All six unit cell parameters must be given regardless of the crystal symmetry.

14-16 The 'INV ' in columns 1-5 indicates that the INV program function will be executed. The ' 2' in columns 9-10 specifies that the inverses for two matrices will be calculated.

B. Program output

1-3 The SYM program function can be used in the routine determination and evaluation of symmetry. For this C-centered cell, the LATTICE program generated a group of 6 symmetry matrices showing that the metric symmetry is rombohedral. The crystal structure was originally reported in a C-centered monoclinic space group. Later, the structure was reanalyzed and republished in a rhombohedral space group.

4-6 The RSS program function may be used to establish the relationship between two cells determined on a diffractometer.

The first input cell (Cell A) was determined on an automated diffractometer, diffraction data were collected, and the structure was solved. The structure solution was not completely successful as there appeared to be an unusual amount of disorder. A cell was determined a second time (second input cell; Cell B) and it was found to have twice the volume of the initial cell. When the data were recollected and the structure was solved on the basis of Cell B, the disorder disappeared.

Cell B was found to be a supercell of Cell A as a matrix relating the two cells has integer elements and a determinant of 2. In this case, a subcell of the correct cell was determined by missing nodes in reciprocal space. This example illustrates how the calculation of derivative lattices may prove useful in routine crystallographic analyses.

7-10 The REL program function can be used to determine derivative subcell/supercell as well as composite relationships between cells. In this example, CELL 1 was determined from a single crystal using an automated diffractometer, while CELL 2 was deduced by indexing a powder pattern.

When determining a cell from powder data using an indexing program, one may obtain a cell that is related to the correct cell, especially if too few lines have been used or if the d-spacings have large experimental errors.

The output for this problem shows that CELL 2 is related to CELL 1 by a matrix whose elements are integers and simple rational numbers. In this case, therefore, the relationship is not that of a subcell or supercell, but is a composite one. The ability to establish such a relationship is very useful when characterizing materials.

11-13 In lattice analyses, it is often necessary to transform one unit cell to another. In this example, the TRANS program function is used to transform the unit cell obtained by powder indexing to the correct cell of the lattice.

14-16 The INV program function calculates the inverses of these matrices.

Appendix

Synopsis of Algorithm to Generate All Converse-Transformation Matrices (H) Relating Two Lattices. The Transformation is Defined by the Equation {Y = (H Matrix) Z}.

Part 1: Find Matrix Triples which Statisfy Transformation of Cell Edges (Only).

--- Generate one at a time all potential matrix triples. Input matrix elements are used to form a row of a transformation matrix. Test each triple as outlined below.

--- Calculate symmetrical dot products for transformed Cell Z. Dot product may be a.a, b.b, or c.c depending on order of matrix row in the final transformation matrix H.

--- Calculate transformed cell edge for cell Z.

--- Test whether matrix triple transforms a-cell edge for Z to Ya within the specified tolerance.

-- If yes, matrix triple is a possible 1st row in a matrix H, save matrix row, actual tolerance, transformed cell edge for Z.

--- Test whether matrix triple transforms b-cell edge for Z to Yb within the specified tolerance.

-- If yes, matrix triple is a possible 2nd row in a matrix H, save matrix row, actual tolerance, transformed cell edge for Z.

--- Test whether matrix triple transforms c-cell edge for Z to Yc within the specified tolerance.

-- If yes, matrix triple is a possible 3rd row in a matrix H, save matrix row, actual tolerance, transformed cell edge for Z.

--- Repeat cycle until all potential matrix triples have been generated and tested. Then go to Part 2 (next page).

Part 2: Starting with Matrix Triples Satisfying Transformation of Cell Edges (For Z to Y), Determine which Combinations also Transform Cell Angles.

--- Generate all combinations of matrix triples for first 2 rows of H Matrix. Test one at a time as outlined below.

--- Calculate gamma for transformed Cell Z and check whether it is within specified tolerances.

--- If yes, then test one at a time all possible 3rd rows with a given row 1 and 2 combination.

-- Determinant of matrix H will be positive--if not check next combination of matrix triples.

-- Calculate alpha for transformed cell Z and check whether it is within specified tolerances.

-- Calculate beta for transformed cell Z and check whether it is within specified tolerances.

-- If alpha and beta are acceptable, then this combination of three matrix triples transforms cell Z to cell Y within the specified tolerances -- assign the elements to matrix H. Output H.

--- Repeat cycle until all possible 3rd rows have been combined with a given row 1 & 2 combination.

--- Repeat cycle until all potential H matrices (combinations of matrix triples from Part 1) have been generated and tested.

In NIST*LATTICE, this algorithm has been encoded in standard, structured FORTRAN. A detailed discussion of the strategy and applications to phase characterization and to the automation of single-crystal diffractometers has been set forth in a Patent Disclosure (Karen, V. L. and Mighell, A.D. (1989) U.S. Patent Application 07/434,383).

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11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)

The NIST*LATTICE program is written in standard FORTRAN and is designed to be used in any analytical laboratory. The software is multifunctional and can be used to analyze various types of lattice relationships. The present version of the program performs several functions including : 1) the determination of symmetry, and the evaluation of experimental error, through Converse-Transformation analysis; 2) the generation of transformation matrices relating any two unit cells; 3) the calculation of the reduced cell of the lattice, and the calculation and reduction of specified derivative supercells and/or subcells; 4) unit cell transformations; and 5) matrix inversions. It is planned to incorporate additional features in forthcoming versions of this program.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

computer program; derivative lattice calculation, latttice relationships, reduced cells; symmetry determination

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